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LIQUID WATER PRODUCTION FROM ATMOSPHERIC SOURCES

ABSTRACT Report documents theoretical analysis of hypothetical liquid desiccant based systems for producing liquid water through collection of atmospheric moisture. Estimates are made of cost, weight, and water production rate for the hypothetical system

NAVAL CIVIL ENGINEERING LABORATORY PORT HUENEME CALIFORNIA 93043-5003

METRIC CONVERSION FACTORS

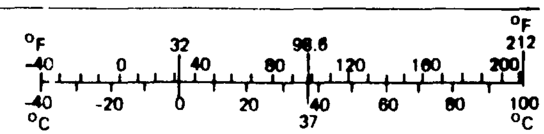
Approximate Conversions to Metric Measures

Symbol	When You Know	Multiply by	To Find	Symbol
		LENGTH		
in	inches	*2.5	centimeters	cm
ft	feet	30	centimeters	cm
yd	yards	0.9	meters	m
mi	miles	1.6	kilometers	km
		AREA		
in^2	square inches	6.5	square centimeters	cm^2
ft^2	square feet	0.09	square meters	m^2
yd^2	square yards	0.8	square meters	m^2
mi^2	square miles	2.6	square kilometers	km^2
	acres	0.4	hectares	ha
		MASS (weight)		
oz	ounces	28	grams	g
lb	pounds	0.45	kilograms	kg
	short tons (2,000 lb)	0.9	tonnes	t
		VOLUME		
tsp	teaspoons	5	milliliters	ml
Tbsp	tablespoons	15	milliliters	ml
fl oz	fluid ounces	30	milliliters	ml
c	cups	0.24	liters	l
pt	pints	0.47	liters	l
qt	quarts	0.95	liters	l
gal	gallons	3.8	liters	l
ft^3	cubic feet	0.03	cubic meters	m^3
yd^3	cubic yards	0.76	cubic meters	m^3
		TEMPERATURE (exact)		
°F	Fahrenheit temperature	5/9 (after subtracting 32)	Celsius temperature	°C

*1 in = 2.54 (exactly). For other exact conversions and more detailed tables, see NBS Misc. Publ. 286, Units of Weights and Measures, Price $2.25, SD Catalog No. C13.10 286.

Approximate Conversions from Metric Measures

Symbol	When You Know	Multiply by	To Find	Symbol
		LENGTH		
mm	millimeters	0.04	inches	in
cm	centimeters	0.4	inches	in
m	meters	3.3	feet	ft
m	meters	1.1	yards	yd
km	kilometers	0.6	miles	mi
		AREA		
cm^2	square centimeters	0.16	square inches	in^2
m^2	square meters	1.2	square yards	yd^2
km^2	square kilometers	0.4	square miles	mi^2
ha	hectares (10,000 m^2)	2.5	acres	
		MASS (weight)		
g	grams	0.035	ounces	oz
kg	kilograms	2.2	pounds	lb
t	tonnes (1,000 kg)	1.1	short tons	
		VOLUME		
ml	milliliters	0.03	fluid ounces	fl oz
l	liters	2.1	pints	pt
l	liters	1.06	quarts	qt
l	liters	0.26	gallons	gal
m^3	cubic meters	35	cubic feet	ft^3
m^3	cubic meters	1.3	cubic yards	yd^3
		TEMPERATURE (exact)		
°C	Celsius temperature	9/5 (then add 32)	Fahrenheit temperature	°F



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Executive Summary

This document summarizes the work performed at the Naval Civil Engineering Laboratory (NCEL) and Solar Energy Research Institute (SERI) under the Independent Exploratory Development (IED) project "Water Production Dehydrator." The purpose of this effort was to assess the feasibility of developing a desiccant system to produce potable water from atmospheric sources that is compatible with military constraints. The goals of this effort were: (1) to examine desiccant technology, investigate methods of using available desiccants to collect atmospheric moisture, (2) develop a conceptual model of a desiccant water production system, and (3) develop a mathematical model to simulate the operation of the conceptual model.

The results show that a desiccant system can produce large quantities of potable water using relatively small amounts of fuel for heat and fan power. A solid desiccant based system, commercially available from Mitsubishi Limited, has produced as much as 3.5 gallons water per gallon fuel burned. Because it appeared that a liquid based system may have greater fuel efficiency and more compact size, a hypothetical system was analyzed. A comparison of the maximum theoretical performance of a liquid desiccant based system versus a solid system showed the liquid system to have 155 percent of the performance potential of the solid system. Based on this analysis, a conceptual design for a liquid desiccant system was developed. The conceptual system includes working fluid (liquid desiccant), absorber, heat exchanger, distillation column, condenser, and subcooler arranged as shown in Figure 1. This system was analyzed using a FORTRAN code developed specifically for this project. The code actually sized the components based on operating conditions and performance requirements. The results are shown in Table 1 and are compared to the performance of the commercial unit.

Table 1. Estimated Performance

	Commercial Unit	Liquid Unit
Water/Fuel Ratio	3.5 gal	7.3 gal
Power	13.3 kW	6 kW
Weight	10,000 lb	4,175 lb
Cost	$100,000	$33,300*

*Components only

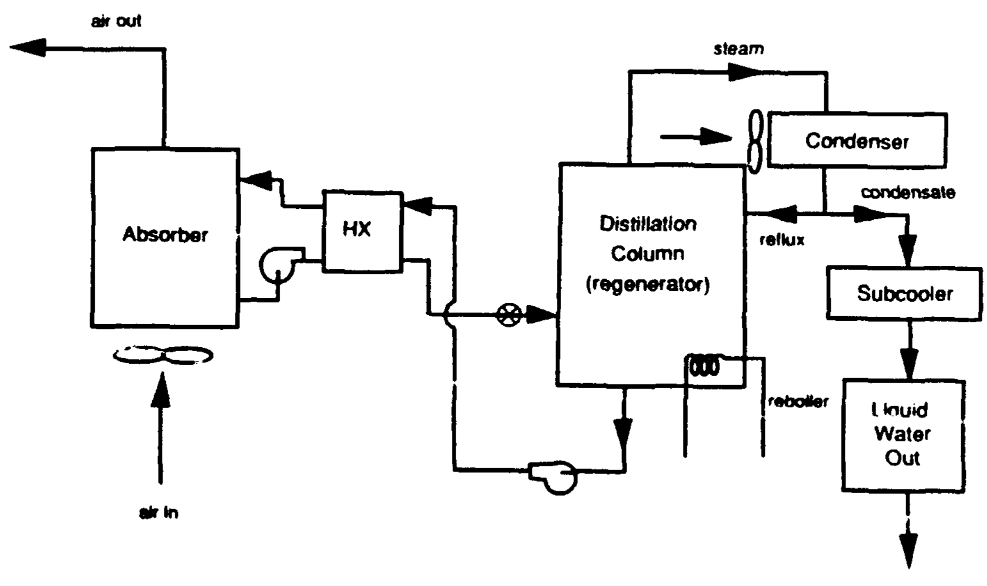

Figure 1. Atmospheric moisture collection system schematic.

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INTRODUCTION

Water is perhaps the most essential requirement for human survival. Particularly in arid climates, water is respected as a life sustaining essential. Even in the most arid climates some moisture always exists in the atmosphere in the form of humidity, even though no surface water may exist. This water is not available directly, i.e., it cannot be simply sponged out of the air and squeezed into a water glass. However, it is possible to remove some of the water by condensing it out of the air through cooling and/or pressurizing. These techniques, when used alone, are energy intensive and are, therefore, not of particular interest. It has been shown (Ref 1) that using a desiccant material, substantial quantities of potable water can be extracted from air with absolute humidity as low as 3 g H_2O/kg. Previous efforts using this technique have focused on using solid desiccants such as silica gel and molecular sieves.

Liquid desiccants are also effective at absorbing moisture and could be used in producing water. While the basic process would be the same with solid or liquid desiccant, the properties of a liquid desiccant allow using equipment that may result in a more compact and energy efficient system then possible when using a solid desiccant.

The focus of this project was using a liquid desiccant (such as triethylene glycol) in an absorption-distillation cycle much like that used in the petroleum refining process. The concept investigated, referred to as the atmospheric moisture collection system (AMOCS), was developed into a conceptual design and analyzed to predict its performance potential. The performance predictions were based on empirical data available in literature (Ref 2, 3, 4, and 5).

BACKGROUND

Humidity is water vapor that exists in air as a result of the stoichastic nature of molecules. At a given temperature, a portion of a set of water molecules existing as water will have enough energy to be liberated from the the rest of the liquid and take on the gaseous vapor form. Concurrently, a certain number of water molecules existing at the vapor state will strike the liquid surface and give up energy to assume the liquid form. Equilibrium is defined as when the rate of liquid to vapor transition is equal to the rate of vapor to liquid transition. Depending on the temperature and pressure, the equilibrium concentration of water vapor above a reservoir of liquid water can be calculated. Thus we have:

$$w = w(T, P) \qquad (1)$$

where: w = absolute humidity (kg H_2O/kg air)
T = absolute temperature (°K)
P = absolute pressure (N/m^2)

The exact relationship between w, P, and T is extremely nonlinear, but can be approximated or looked up in psychrometric charts such as shown in Figure 2.

Some of this moisture can be condensed (forced to assume the liquid form) by lowering the temperature of the vapor/air mixture. Unless a low temperature heat sink is available, however, this process requires the expenditure of mechanical work. Furthermore, the heat transfer coefficients for condensation of water vapor in the presence of air are undesirably low. If water is to be removed from air with minimum work requirements and maximum heat transfer coefficients, another technique must be used.

One technique that appears promising is a combination of a desiccant dehumidifier, a desiccant regenerator, and a condenser. A desiccant is a material that has an extremely high affinity for water vapor. The desiccant will absorb water vapor from the air until the desiccant is saturated with water. Desiccant saturation occurs when the desiccant moisture density is in equilibrium with the absolute humidity. The saturation point, measured in mass of water per mass of dry desiccant, is a function of desiccant chemistry, temperature, and pressure. Thus we have:

$$v = v(T, P) \qquad (2)$$

where: v = equilibrium desiccant moisture density (lbm H_2O/lbm desiccant)

The exact relationship between temperature, pressure, and equilibrium desiccant moisture density is highly nonlinear. Equilibrium curves are available in the literature for many desiccants. Curves for triethylene glycol, the desiccant chosen for this study, are shown in Figure 3.

Although the use of desiccants permits air dehydra-

n without the expenditure of mechanical work (other ın that required to move the air), the water is still not ıilable in liquid form. It has, however, been isolated m the air. To remove the water from the saturated des-ant, the desiccant must be heated. This lowers the ɪilibrium moisture density of the desiccant and vapor-s the water into steam. This process of stripping the ɪiccant of its water requires heat, but no thermodynamic ɪrk. It may appear now that the processes of saturating : desiccant and then stripping it have only resulted in a urn to the original state, plus the expenditure of some at. The important result is that the water is now in the m of steam rather than water vapor mixed with air. The gher heat transfer coefficients obtained when condensing ıter vapor isolated from air translates into much smaller ndenser area requirements. Further, the steam tempera-e is well in excess of ambient, so natural cooling may be ed to condense the steam to liquid water.

ECHNICAL APPROACH

This project was divided into three distinct phases:) literature search, (2) conceptual design, and (3) concep-ıl system performance analysis. Descriptive details of ch phase are included in the following paragraphs.

terature Search

The purpose of the literature search was to establish : current state of air dehydration technology as well as view any prior work in atmospheric water collection. It ıs immediately clear that desiccants were by far the most pular choice for air dehydration. However, nearly all the plications first reviewed were concerned with using solid siccants to dehumidify airstreams. References 6, 7, 8, d 9 discuss and analyze various techniques for using id desiccants, primarily silica gel, for dehumidifying an stream. Typically, these applications are part of a solar wered air-conditioning system. The solar energy was ed directly to heat and dry (regenerate) the desiccant. A nple analysis indicates that the collector size for solar generation of desiccant in a water production system ɪuld be impractical for a mobile system. This is due to : high latent heat of vaporization of water when con-nsed on a desiccant, the relatively low power level of ar insolation, and the need to produce relatively large antities of water. Therefore, these references were of pe-heral interest.

Liquid desiccant based air-conditioning systems were o reviewed. References 10 and 11 discuss various hniques for regenerating liquid desiccants such as lith-n chloride and triethylene glycol. The major thrust of these analyses was to regenerate the desiccant without regard to collecting the moisture (as was that of the solid desiccant research). These references were also of only limited interest.

The natural gas industry has been using various liquid desiccants to dehydrate natural gas for many years. This application was clearly the most directly applicable to the current project. A thorough review of the industry's publications revealed a wealth of knowledge in the form of empirical desiccant regeneration and absorption data (Ref 2, 3, 4, and 5) and design data. Reference 12 also provided industry standard design guidelines for direct contact gas coolers and condensers.

In the course of the literature search, a commercial device called the Mobile Water Collection System (MWCS) built by Mitsubishi Electric, Ltd was identified. A review of MWCS literature showed that it was based on a solid desiccant operating in a batch mode. Its performance is quoted as 3.5 gallons water per gallon of fuel burned and 400 gallons of water produced in a 24-hour period. Thus, the feasibility of producing water from atmospheric sources is demonstrated. The goal, therefore, of the conceptual system design for AMOCS was to determine whether there was potential capability to perform substantially better than the commercial system.

Conceptual Design

The original concept of the AMOCS was based on a solar regenerated solid desiccant. As described previously, solar regeneration is impractical for this type of application. Further, because the liquid desiccant systems had been so successfully used in the natural gas industry, liquid desiccant was selected as the basis for the conceptual design. Finally, the substantial performance improvement being sought required a departure from previous concepts. Because the commercial MWCS was based on a solid desiccant, and there was no evidence that liquid desiccant systems had been considered, a liquid based system approach was selected.

An AMOCS can operate in either a continuous or batch process mode. The solid based MWCS operates in a batch process mode only. While one adsorption chamber is being regenerated and producing steam for condensation, the other chamber is being saturated. Once saturation and regeneration are complete, the processes are switched. The chamber that has been fully regenerated is now switched to an adsorption mode and the fully saturated chamber is regenerated. The system schematic is shown in Figure 4. Similarly, a liquid desiccant based system can operate in a batch process mode or a continuous mode. The continuous process mode was selected for the conceptual design based on the experience of the natural gas industry.

A continuous process liquid desiccant based AMOCS requires five major components. These components are shown in the schematic of the conceptual design in Figure 1. The absorber exposes the lean (water poor) desiccant to the ambient air. Some of the moisture in the air (humidity) is absorbed by the desiccant and its latent heat of vaporization is released. The desiccant, now rich (water rich), is pumped through the heat exchanger where it receives heat from the lean desiccant on its way to the absorber. From the heat exchanger, the rich desiccant is fed to the regenerator where it is heated and stripped of most of its water. The now lean desiccant is then fed back through the heat exchanger and on to the absorber. This constitutes the continuous process water collection cycle. The water stripped from the desiccant in the regenerator is now in the form of steam. The steam is directed to a condenser to liquify the steam using forced air cooling. The condensate leaving the condenser is still quite hot ($\approx$100°C) and is cooled further by a subcooler also using forced air cooling.

Conceptual System Performance Analysis

Selecting the components for the conceptual design was based on natural gas industry standards. Several choices were available for the absorber and regenerator. Baffle tray columns, spray chambers, packed columns, and pipeline contactors are valid options. Because of the volume of air that must be exposed to the desiccant in the absorption process and the tendency for sprays to become entrained, the spray chamber and pipeline contactor options were eliminated. Packed columns were selected over baffle tray columns due to their higher spatial efficiency. A packed column was selected for the regenerator for similar reasons. The heat exchanger was a simple plate counter flow device. The condenser and subcooler were simple air cooled heat exchangers.

Desiccant. Selecting the desiccant for the conceptual design required reviewing several compounds currently used in industry. Of particular concern was the toxicity of the desiccant to humans upon ingestion. It was anticipated that trace quantities of the desiccant would be left in the condensate after distillation. Triethylene glycol was selected based on the availability of hygroscopic data and low toxicity characteristics.

To simplify later analysis, a design point was selected and a conceptual design was developed around that point. The design conditions were:

T_{DB} = 30°C
RH = 30%
(w = 0.0078 kg H_2O/kg air)
Output = 10 gallons per hour

where: T_{DB} = Temperature dry bulb
RH = Relative humidity

Distillation Columns. Once the component types had been specified and the design point selected, the components could be sized and priced. The distillation column requirements could be analyzed using either a continuous exchange model or an equilibrium tray model. The equilibrium tray technique was selected due to the simplicity of the method and the lack of requirement for mass and heat transfer coefficient data. A computer routine based on the equilibrium tray approach using the McCabe-Thiele graphical method was used to model the distillation column. The distillation model analysis is shown in Appendix A. The program "DIST5.FOR," written in Microsoft FORTRAN is also listed in Appendix A.

The final distillation column design values were:

Theoretical Trays	= 3
Equiv. Height Packing	= 28 in. (Flexipack 1Y)
Column Height	= 84 in.
Column Diameter	= 6 in.
Pressure Drop	= 0.84 in. H_2O
Cost	= \$4,000 (including packing)

The other parameters associated with the distillation column that had to be calculated were the distillation peak temperature, reflux ratio, and the reboiler load. The peak allowable temperature was 375°F, the maximum temperature of triethylene glycol before disassociation occurs. This maximum distillation temperature also restricts the level of regeneration that can be achieved at atmospheric pressure. The maximum purity of desiccant leaving the distillation column was, therefore, calculated to be 98 percent (2 percent water). The purity of the steam leaving the distillation is controlled by the reflux ratio (portion of condensate returned to distillation column divided by the portion removed from the desiccant cycle). Based on the toxicity levels for triethylene glycol, the corresponding water purity level must be greater than 99.99 percent (less than 0.01 percent triethylene glycol). This requires a reflux ratio of at least 0.27.

Absorption Column. The absorption column was designed using the same technique used for the distillation column. A separate computer routine was written to model the absorption column and is listed in Appendix B. The final design values for the absorption column were:

Theoretical Trays	=	1
Equiv. Height Packing	=	48 in. (Structured Flexipak Type 2)
Column Height	=	48 in. (external = 8 feet)
Column Diameter	=	48 in. (external = 5 feet)
Pressure Drop	=	2.0 in. H_2O
Cost	=	$20,000

Heat Exchanger. The heat exchanger was de- ɔed based on the temperatures of the the saturated, cool iccant coming from the absorption column and the hot, pped desiccant coming from the distillation column and desiccant flow rate. Assuming an overall heat transfer fficient of 40 Btu/hr/ft², approximately 1,050 ft² of hanger area are required. A plate type heat exchanger neet this requirement was:

Size	= 36 x 24 x 24 in.
Weight	= 400 lb
Cost	= $3,000

Condenser. The condenser was designed based on incoming steam flow rate and the ambient (design nt) air temperature. Its heat load was calculated to be ,000 Btu/hr and an air cooled heat exchanger was:

Size	= 66 x 39 x 27 in.
Weight	= 385 lb
Cost	= $1,470

Subcooler. The subcooler was designed based on temperature of the incoming condensate and a desired put temperature of 96°F. This output temperature was cted as the lowest practical temperature for forced air ling. Its heat load was calculated to be 12,000 Btu/hr was:

Size	= 47 x 22 x 22.5 in.
Weight	= 156 lb
Cost	= $650

forced air cooler could be eliminated in favor of a ling tank if time is available for natural convection ling.

Waste Heat. During the conceptual design, it was gested that waste heat from a generator or other engine ht be available to heat the desiccant for regeneration. determine the feasibility of this concept, the heat avail- from engine exhaust was compared to the heat re- ements of this system. The exhaust temperature from a cal turbo-charged diesel engine is approximately 750°F. at exhaust stream is cooled to 400°F, the engine pro- ed roughly 1,000 Btu/hr/hp. Based on a need for 145,500 Btu/hr in the reboiler, a 150-hp engine should supply enough heat to regenerate the desiccant. Additional heat may be available from the engine cooling jacket.

RESULTS

Once all the components had been sized and selected, a system analysis could be performed. Based on the design point operation, the system was calculated to perform as:

Water Output = 10.7 gph

Power Requirements

Desiccant Loss	= 0.4 gal 1 day (24 hr)
Reboiler	= 1.5 gal fuel/hr
Absorption Column Fan	= 3.0 kW
Condenser Fan	= 1.6 kW
Subcooler Fan	= 0.83 kW
Desiccant Pump	= 0.10 kW
Total	= 5.5 kW + 1.5 gal fuel/hr

The conceptual system cost and weight breakdown is:

Item	Weight (lb)	Cost ($)
Distillation Column	250	4,000
Absorption Column	1,500	20,000
Reboiler	1,400	3,670
Heat Exchanger	400	3,000
Condenser	385	1,470
Subcooler	160	650
Desiccant Pumps (2)	80*	510*
Total	4,175	33,300

*Each pump weighs 40 pounds and costs $205.00

At this point in the analysis, it is possible to compute the effective ratio of water produced to fuel consumed. Assuming a heating value of 135,000 Btu per gallon of fuel and 20 percent heat loss, the ratio is 7.3 gallons H_2O produced per 1 gallon of fuel burned. Compared to the ratio for the commercially available MWCS solid desiccant system, this result is extremely favorable even though it is based on relatively conservative assumptions. Moreover, the electric power requirement of this theoretical liquid desiccant system is less than half that of the equivalent size MWCS. Rough estimates of size and weight of the liquid system suggest that a 10-gallon per hour device could be built within a 8- by 8- by 10-foot frame (HALFCON) and would weigh less than 5,000 pounds. The cost

of manufacturing a liquid based system depends heavily on the quantity produced. In 1986, the estimated costs of components for the system, if purchased separately, were $33,300.

Perhaps the single greatest advantage of using liquid desiccant is the greater potential water production rate for a given system weight. Dividing the estimated water produced per hour by the system weight, we find the specific water productivity is 2.59×10^{-3} gallon of water per hour per pound. The MWCS solid desiccant system, on the other hand, has a specific productivity of 5.55×10^{-4} gallons of water per hour per pound. The theoretical liquid system has nearly a five-fold advantage in specific productivity.

The unique capability of the desiccant based water collection system, solid or liquid based, is its ability to produce water without a feed water source. Although other water purification systems such as reverse osmosis require a feed water source, a comparison of their performance with a desiccant system might be interesting. An existing reverse osmosis system is the Marine Corps' 600 gallons per hour (GPH) Reverse Osmosis Water Purification System (ROWPU). As its name implies, it produces 600 GPH of purified water from salt water. It can produce 1200 GPH from fresh water sources. The device weighs approximately 7300 pounds and requires a 30 kW external power supply. It fits within a HALFCON frame. Its specific productivity (system weight divided by water production rate) ranges from 12.2 to 6.1 pounds per gallon of water per hour. Clearly, the capability to produce water without a feed water source carries with it a severe weight penalty.

CONCLUSIONS

The effort documented here has attempted to assess the feasibility of developing a mobile desiccant system to produce potable water for military use. There is a commercial system based on a solid desiccant that is capable of producing 3.5 gallons of water per gallon of fuel burned. This study was focused on investigation of liquid desiccant based systems. A liquid desiccant system was conceptualized and analyzed using fundamental engineering analysis and computer models. The results of the liquid system analysis indicate that substantially higher efficiency and specific productivity can be achieved by the liquid system.

Further work is necessary before exploratory development is completed. First, more flexible models must be developed. Improved models will permit examination of the system and the impact of the following variables:

1. Operation in off-design conditions
2. Simulation of different desiccants
3. Vacuum distillation of desiccant
4. Higher desiccant flowrates

RECOMMENDATIONS

If the improved computer models support the indications of the study contained herein, a process model of the conceptual system should be developed and tested. Assuming the process model further supports the results of this study, NCEL recommends that an advanced development model of the conceptual liquid based system be fabricated and tested to verify the performance predictions.

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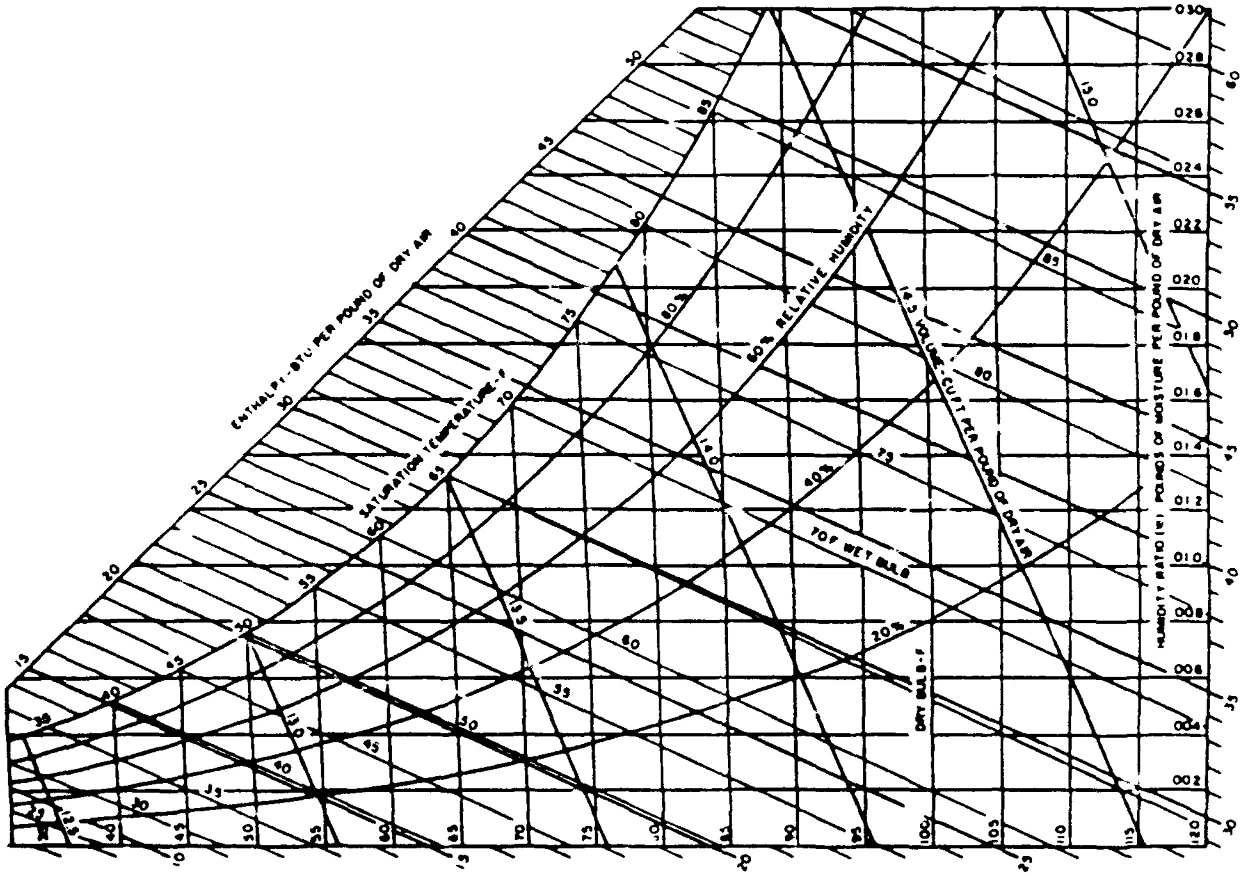

Figure 2. Psychrometric chart.

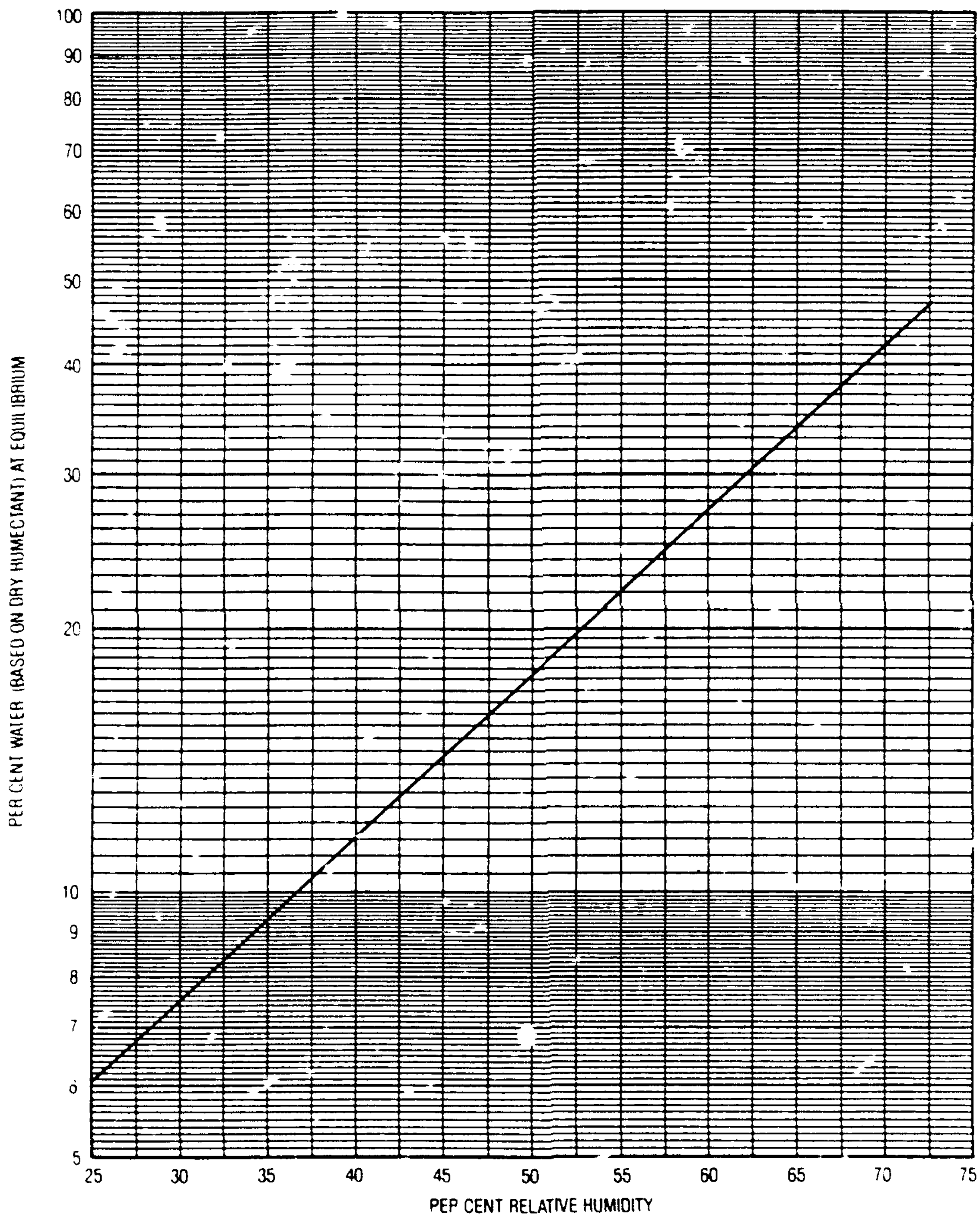

Figure 3. Hygroscopicity of triethylene glycol at 70° to 80°F.

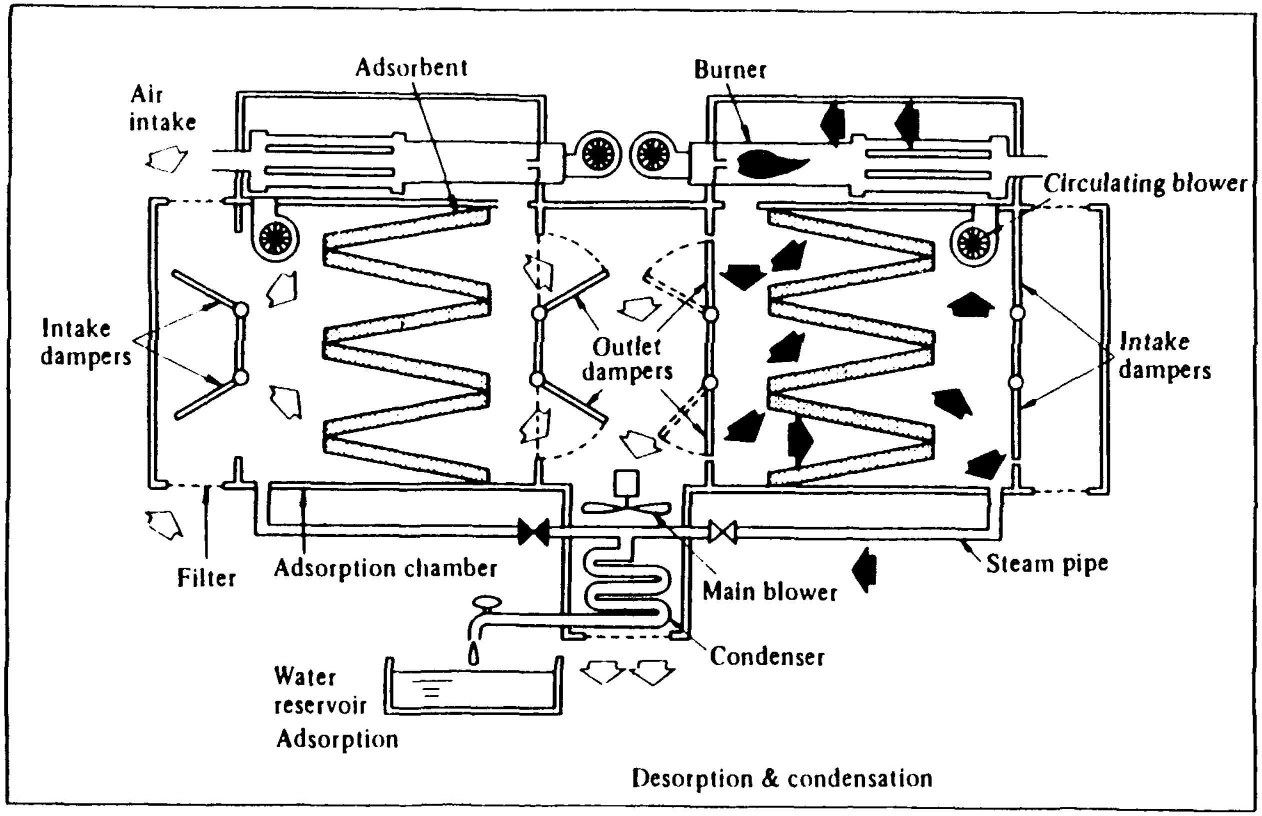

Figure 4. Mitsubishi mobile water collection system schematic (batch process).

Appendix A

DIST!LLATION COLUMN ANALYSIS

The distillation column is modeled using the equilibrium tray approach (see Figures A-1 and A-2):

where: d = molar flow rate of distillate
X_d = mole fraction of water in distillate
Q_c = condenser heat
r = reflux rate
b = molar flow rate of bottom product
X_b = mole fraction of water in bottom product
f = molar flow rate of feed product
X_f = mole fraction of water in feed product
Q_{RB} = reboiler heat
V = total molar gas flow rate
L = total molar liquid flow rate
Y = mole fraction of steam in gas
X = mole fraction of water in liquid
P = refers to any plate

The following are known:

d = 5.2 LB-moles/hr: determined from water requirement: 200 gal/day x 1 day/18 hrs x 8.34 lb/gal = 92.7 lb/hr or 5.2 LB-moles/hr

X_d = 0.99992: from purity requirement

X_b = 0.145 (98%): determined from maximum allowable boiling temperature for glycol - 375°F

X_f = 0.318 (95%): based on glycol flow of 3 gal per lb H_2O absorbed

f = 25.2 LB-moles/hr, b = 20.0 LB-moles/hr: determined from simultaneous solution of total mass balance and water balance:

$$b = f - d$$

$$X_b b = X_f f - X_d d$$

$$Q_c = (d + r)\, h_{f_g}$$

Unknowns: $V_p, L_{p+1}, Y_p, X_{p+1},$

H_p, h_{p+1}, N, Q_{RB}

SOLUTION PROCEDURE

1. $Y_1 = f(X_1)$ Equilibrium

   $Y_p = f(X_p)$

2. $H_p = f(Y_p)$

3. Assume $X_{p+1}, h_{p+1}, = f(X_{p+1})$

4. Solve for V_p and L_{p+1} from two simultaneous equations:

   $V_p H_p = L_{p+1} h_{p+1} + h_d d + Q_c$ energy balance

   $V_p - L_{p+1} = d$ mass balance

5. Determine x_{p+1} from

   $V_p Y_p = L_{p+1} X_{p+1} + X_d d$ water balance

6. Substitute X_{p+1} for value assumed, iterate to convergence

7. Move to next plate up until X_{p+1} / X_d

RESULTS (see Figure A-2)

```
C This program simulates a binary distillation column

      PROGRAM DISTILL
      REAL L(100)
      DIMENSION V(100), X(100), X2(100), Y(100)
      DIMENSION HVAP (100), HLIQ(100), TDIST(100)
      KDFLAG = 0
      XD = .9992
      FEED = 25.2
      XF = .318
      XB = .1445
      DIST = FEED*(XF - XB)/(XD - XB)
      STEPCON = .001
      HVAPD = 20709
      HLIQD = 3242
      ICOUNT = 1
```

```
BETA = .05
I = 1
X(1) = XB
CALL EQUIL(X(1),Y(1))
RRMIN1 = (XD - Y(1)/(XD - X(1))
RRMIN = RRMIN1/(1 - RRMIN1)
PRINT, "ENTER REFLUX RATIO:"
INPUT, RR
REFLUX = RR*DIST
QC = (DIST+REFLUX)*(HVAPD-HLIQD)
X(2) = .80
I FORMAT (1X,"PLATE","Y","X","T","V","1","L")
PRINT 50
)0 CONTINUE
IF (ICOUNT.GT 2000) THEN PRINT, "NOT CON-
ERGING.  TRY AGAIN WITH A          HIGHER
EFLUX."
GOTO 160
ELSE
  CONTINUE
ENDIF
IF (ICOUNT.GT.500) BETA = .2
IF (ICOUNT.GT.1000) BETA = .4
CALL SATVAP(Y(I),HVAP(I),TDIST(I))
CALL SATLIQ(X(I+1),HLIQ(I+1))
L(I+1) = (QC - (HVAP(I)-HLIQ)*DIST)/(HVAP(I) -
LIQ(I+1))
V(I) = L(I+1) + DIST
X2(I+1) = (V(I)*Y(I) - XD*DIST)/L(I+1))
110 FORMAT (1X, "X2 = ",F8.5)
PRINT 110, X2(I+1)
IF (X2(I+1).GT.0.99) STEPCON = .00001
IF (X2(I+1).LE.0.99) STEPCON = .001
IF (ABS(X2(I+1)-X(I+1).GT.STEPCON) THEN
  X(I+1) = X(I+1) + BETA*(X2(I+1) - X(I+1))
  ICOUNT = ICOUNT + 1
  GOTO 100
ELSE
  CONTINUE
ENDIF
IF (X(2).GT.1.0) THEN
  PRINT, "X GREATER THAN 1.  USE A
  HIGHER REFLUX."
  GOTO 160
ELSE
  CONTINUE
ENDIF
ICOUNT = 1
BETA = .05
STEPCON = .001
5 FORMAT (1X, I3, F10.5, F8.5, F6.1, F7.2, F7.2)
PRINT 125, I, Y(I), X(I+1), TDIST(I), V(I), L(I+1)
IF (X(I+1).GE.XD.AND.KDFLAG.EQ.0) THEN
  DPLATES = I - 1 + (XD-X(I)/(X(I+1)-X(I))
  KDFLAG = 1
  GOTO 130
ELSE
  CONTINUE
ENDIF
130 IF (XD.GT.X(I+1)) THEN
  I = I+1
  CALL EQUIL(X(I),Y(I))
  X(I+1) = X(I)
  GOTO 100
ELSE
  CONTINUE
ENDIF
PRINT
150 FORMAT (1X, "NUMBER OF THEORETICAL
PLATES = ", F6.2)
PRINT 150, DPLATES
PRINT
160 END
SUBROUTINE EQUIL (V,S)
REAL X(25),Y(25),BY(25),CY(25),DY(25)
REAL S, U, V, SEVAL
CHARACTER FLAG*4
INTEGER I, N
DATA X/0.000,
.05,.10,.15,.20,.25,.30,.35,.40,.45,.50,.55,.60,.65,
*.70,.75,.80,.85,.875,.90,.933,.95,.975,.99,1.0/
DATA Y/0.0,.00024,.00072,.00167,.00286,
.00406,.00525,.00668, *.00835,.01026,.01241,
.01456,.01694,.01957,.0227,.029,.044,.079, *.105,
.149,.255,.352,.585,.805,1.0/
N=25
IF (FLAG .EQ. 'DONE') GO TO 2
CALL SPLINE (N, X, Y, BY, CY, DY)
FLAG = 'DONE'
2 U = 1.0 - V
S = 1.0 - SEVAL (N, U, X, Y, BY, CY, DY)
RETURN
END
C
SUBROUTINE SPLINE (N, X, Y, BY, CY, DY)
INTEGER N,NM1,IB,I
REAL X(N),Y(N),BY(N),CY(N),DY(N)
REAL TY
NM1=N-1
IF (N .LT. 2) RETURN
IF (N .TL. 3) GOTO 50
DY(1) = X(2)-X(1)
CY(2) = (Y(2)-Y(1))/DY(1)
DO 10 I=2, NM1
  DY(I) = X(I+1)-X(I)
  BY(I) = 2.*(DY(I-1)+DY(I))
  CY(I+1) = (Y(I+1)-Y(I))/DY(I)
  CY(I) = CY(I+1)-CY(I)
```

```
10 CONTINUE
      BY(1) = -DY(1)
      BY(N) = -DY(N-1)
      CY(1) = 0.
      CY(N) = 0.
      IF (N .EQ. 3) GO TO 15
      CY(1) = CY(3)/(X(4)-X(2))-CY(2)/)X(3)-X(1))
      CY(N) = CY(N-1)/X(N)-X(N-2))-CY(N-2)/(X(N-
       1)-X(N-3))
      CY(1) = CY(1)*DY(1)**2/(X(4)-X(1))
      CY(N) = -CY(N)*DY(N-1)**2/(X(N)-X(N-3))
15 DO 20 I=2,N
      TY = DY(I-1)/BY(I-1)
      BY(I) = BY(I)-TY*DY(I-1)
      CY(I) = CY(I)-TY*CY(I-1)
20 CONTINUE
    CY(N) = CY(N)/BY(N)
    DO 30 IB = 1,NM1
      I = N-IB
      CY(I) = (CY(I)-DY(I)*CY(I+1)/BY(I)
30 CONTINUE
    BY(N) = (Y(N)-Y(NM1))/DY(NM1) + DY(NM1)
      *(CY(NM1)+2.*CY(N))
    DO 40 I = 1,NM1
      BY(I) = (Y(I+1)-Y(I)/DY(I) - DY(I)
       *(CY(I+1)+2.*CY(I))
      DY(I) = (CY(I+1)-CY(I))/DY(I)
      CY(I) = 3.*CY(I)
40 CONTINUE
    CY(N) = 3.*CY(N)
    DY(N) = DY(N-1)
    RETURN
50 BY(1) = (Y(2)-Y(1))/(X(2)-X(1))
    CY(1) = 0.
    DY(1) = 0.
    BY(2) = BY(1)
    CY(2) = 0.
    DY(2) = 0.
    RETURN
    END
C
C
    REAL FUNCTION SEVAL (N,U,X,Y,B,C,D)
    INTEGER N
    REAL U, X(N), Y(N), B(N), C(N), D(N)
    INTEGER I, J, K
    REAL DX
    DATA I/1/
    IF (I .GE. N) I = 1
    IF (U .LT. X(I)) GO TO 10
    IF (U .LE. X(I+1)) GO TO 30
10 I = 1
    J = N+1
20 K = (I+J)/2
      IF (U .LT. X(K)) J = K
      IF (U .GE. X(K)) I = K
      IF (J .GT. I+1) GO TO 20
30 DX = U-X(I)
      SEVAL = Y(I)+DX*(B(I)+DX*(C(I)+DX*D(I)))
      RETURN
      END
      SUBROUTINE SATLIQ (V,HLIQ,S)
      REAL X(25),TEMP(25),BT(25),CT(25),DT(25)
      REAL S,U,V,KEL,HLIQ,A,B,C,D,E,HH20,
        HTEG,HTSOLN
      CHARACTER FLAG*4
      DATA X/0.000,.05,.10,.15,.20,.25,.30,.35,.40,.45,
        .50,.55,.60,.65, *.70,.75,.80,.85,.875, .90,.933,
        .95,.975,.99,1.0/
      DATA TEMP/0.0,.00309,.00926,.02160,.03704,
        .05247,.06790,.08642,
      *.10802,.13272,.16049, .18827,.21914,.25309,
        .29321, .34568,.41975,
      *.51852,.57099,.62963,.72531,.78395,.87963,
        .95062,1.0/
      N=25
      IF (FLAG .EQ. 'DONE') GO TO 2
      CALL SPLINE (N, X, TEMP, BT, CT, DT)
      FLAG = 'DONE'
2 U = 1.0 - V
      S = 324.0 * SEVAL (N, U, X, TEMP, BT, CT, DT)
        + 212.0
      KEL = (S-32.)*5/9 + 273.15
      DATA A/5.31409/,B/-.00720017/,C/.0000114153/
      HH20 = V*(A*(KEL-273.15) + B/2.*(KEL**2-
        273.15**2)
    * +C/3.*(KEL**3-273.15**3))*7.7546
      DATA D/1.538OE5/,E/5.87E2/
      HTEG = U*(D*(KEL-273.15) + E/2*(KEL**2-
        273.15**2))*4.3033E-4
      DATA HTSOLN/1549.72/
      IF (V .GT. 0.7) HTSOLN=0.0
      HLIQ = HH20 + HTEG - V*HTSOLN
      RETURN
      END
C
      SUBROUTINE SATVAP (V,HVAP,S)
      REAL Y(25),TEMP(25),BT(25),CT(25),DT(25)
      REAL S,U,V,HVAP,KEL,A,B,C,D,E,F,G,H,I,J
    * H20HTVAPN,TEGHTVAPN,HH20,HTEG,TCRIT
      CHARACTER FLAG*4
      DATA Y/0.0,.00024.,00072,.00167,.00286,.00406.,
        00525,.00668,.00835,.01026,.01241,.01456.,
        01694,.01957,.0227,.029,.044,.079,
   * .105,.149,.255,.352,.585,.805,1.0/
      DATA TEMP/0.0,.00309,.00926,.02160,.03704,
        .05247,.06790,.08642,
      *.10802,.13272,.16049,.18827,.21914,.25309,.29321,
```

```
     .34568,.41975
   *.51852,.57099,.62963,.72531,.78395,
     .87963,.95062,1.0/
   N=25
   IF (FLAG .EQ. 'DONE') GO TO 2
   CALL SPLINE (N, Y, TEMP, BT, CT, DT)
   FLAG = 'DONE'
U = 1.0 - V
FORMAT (F12.3)
   S = 324.0 * SEVAL (N, U, Y, TEMP, BT, CT, DT)
     + 212.0
   KEL = (S-32.)*5/9 + 273.15
   H20HTVAPN = (2652.15+.616305*KEL-4.4788E-
     3*KEL**2)*7.7546
   DATA F/1.3088E8/,G/4.60E-1/,TCRIT/700.0/
   TEGHTVAPN = (F*(1.-KEL/TCRIT)**G)
     *4.3033E-4
   DATA A/5.31409/,B/-7.20017E-3/,C/1.14153E-5/
   HH20 = V*(A*(KEL-273.15) +B/2*(KEL**2-
   273.15**2)
   * +C/3*(KEL**3-273.15**3))*7.7546 +
     V*H20TVAPN
   DATA D/1.538E5/,E/5.87E2/
   HTEG = U*(D*(KEL-273.15) + E/2*(KEL**2-
     273.15**2))*4.3033E-4
   * + U*TEGHTVAPN
   HVAP = HH20 + HTEG
   RETURN
   END
```

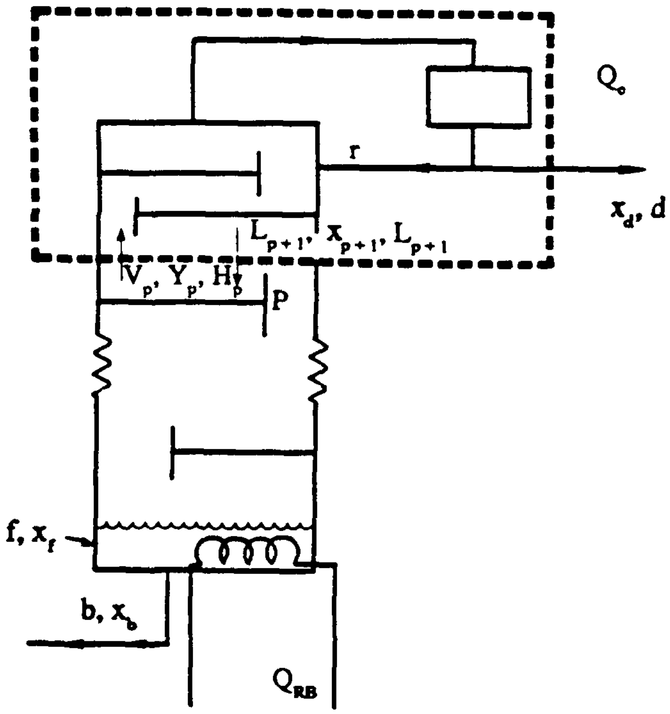

Figure A-1. Distillation column.

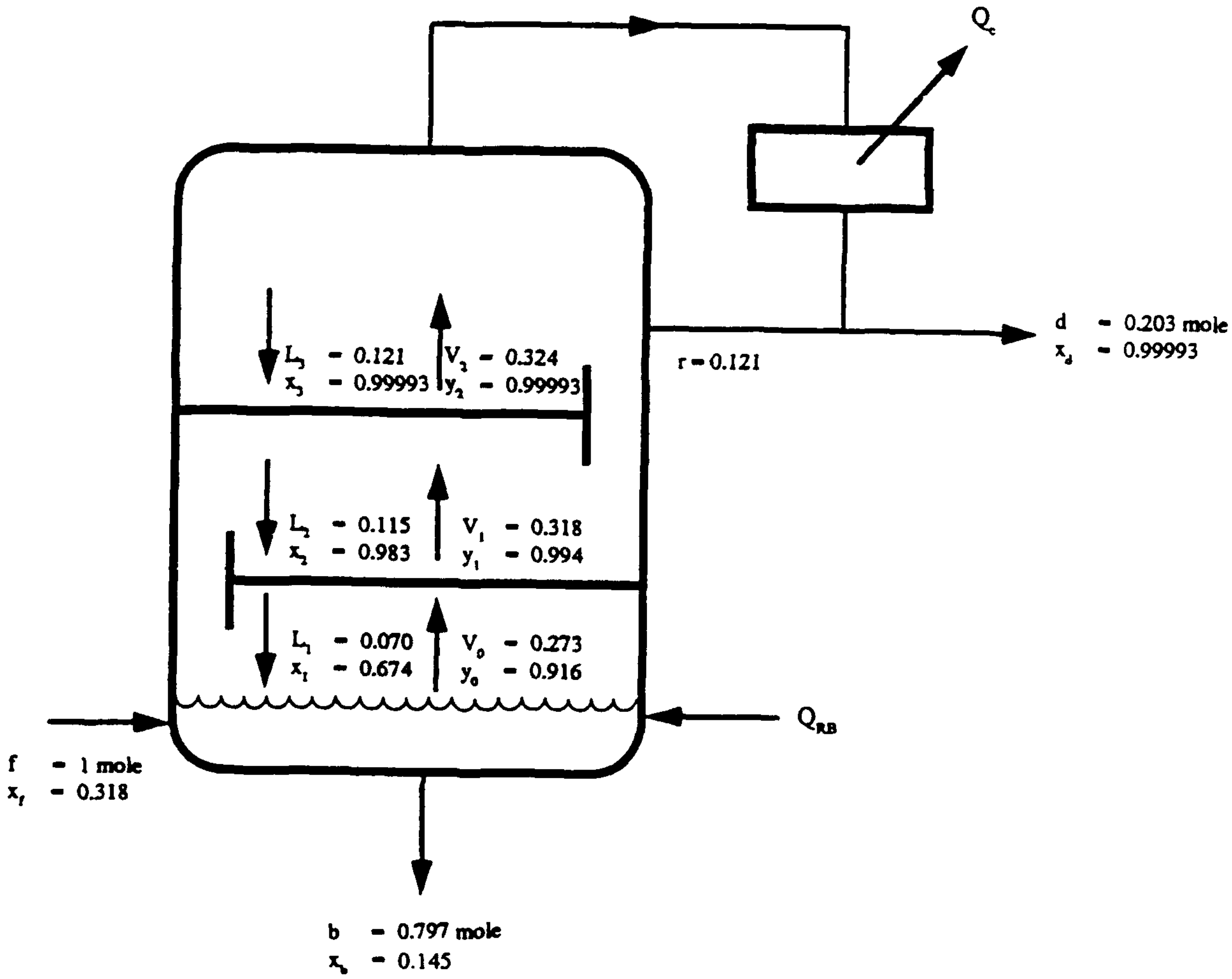

Figure A-2. Equilibrium tray model.

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Appendix B

ABSORBER ANALYSIS

The absorber column is modeled using the equilibrium tray approach (see Figure B-1):

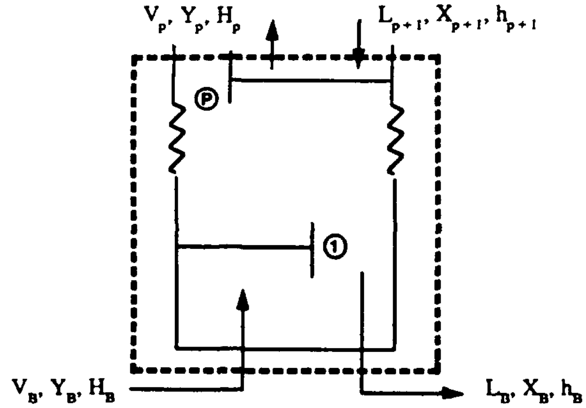

Figure B-1. Absorber column.

where: V = total molar gas flow rate
Y = mole fraction of steam in gas
H = inlet vapor enthalpy for gas
L = total molar liquid flow rate
X = mole fraction of water in liquid
h = enthalpy of water in liquid at inlet

where: p = any plate
B = the bottom of the column
N = number of plates

Known: V_B, Y_B, H_B, L_B, X_B

Unknowns: $V_p, Y_p, H_p, L_{p+1}, X_{p+1}, h_{p+1}, h_B, N$

SOLUTION PROCEDURE

1. Assume T_{LIQ-B} h_B

2. $Y_1 = f(X_b)$(equilibrium)

   $Y_p = f(X_p)$

3. $V_p = \dfrac{(1 - Y_B)}{(1 - Y_p)} V_B$ —— Mass balance on air

4. $H_1 = f(Y_1, V_1, T_{LIQ-B})$

   $H_p = f(Y_p, V_p, T_p)$

5. $L_{p+1} = V_p + L_B - V_B$ —— Total mass balance

6 $X_{p+1} = (X_B L_B + Y_p V_p - Y_B V_B)/L_{p+1}$ —— Water balance

7. $h_{p+1} = (L_B h_B + V_p H_p - V_B H_B)/L_{p+1}$ —— Energy balance

8. $T_{p+1} = f(h_{p+1}, L_{p+1}, X_{p+1})$

9. Repeat above for each tray

When x_T is reached, check T_{LIQ} against known value; if necessary, repeat calculations for different T_{LIQ-B}

```
PROGRAM ABSORB
REAL LA (100)
REAL LB
DIMENSION VA(100), XA(100), YA(100), T(100)
DIMENSION HAIR (100), HLIQ(100)
KFLAG = 0
LB = 25.2
LA(1) = LB
PRINT, "CHOOSE ONE OF THE FOLLOWING:"
PRINT
PRINT
PRINT, "1-THERMAL EQUILIBRIUM (DEFAULT)"
PRINT
PRINT, "2-ISOTHERMAL"
PRINT
INPUT, TFLAG
PRINT
PRINT, "ENTER AIR FLOW RATE IN LB-MOLES/
  HOUR:"
INPUT, VAIRIN
```

```
PRINT,
PRINT, "ENTER EXIT TEMPERATURE OF
   LIQUID IN DEGREES F:"
INPUT, TBOT
HLIQB - 3645.6
PRINT, "ENTER INLET AIR HUMIDITY RATIO:"
INPUT, W
YDUM = 1.6092*W
YAIRIN = YDUM/(1+YDUM)
PRINT, "ENTER INLET AIR TEMPERATURE IN
   DEGREES F:"
INPUT, TAIRIN
PRINT
PRINT, "ENTER COLUMN PRESSURE IN
   ATMOSPHERES:"
INPUT, P
YAIRIN = YAIRIN*P
CALL mixENTH(YAIRIN, TAIRIN, HAIRN)
XT = .1445
XEND = .020
FINCON = .0001
   I = 1
   XB = .3182
   XA(1) = XB
   T(1) = TBOT
50 FORMAT(1X,'PLATE','YA','XA','T','V,'1','L')
PRINT 50
100 CALL EQUILA (XA(I),t(i),YA(I))
   YA(I) = YA(I)*P
   VA(I) = (VAIRIN - YAIRIN*VAIRIN)/(1 - YA(I))
      CALL mixENTH(YA(I),T(I),HAIR(I))
   LA(I+1) = VA(I) + LB - VAIRIN
   XA(I+1) = (XB*LB + YA(I)*VA(I) -
      YAIRIN*VAIRIN)/LA(I+1)
   HLIQ(I+1) = (LB*HLIQB + VA(I)*HAIR(I) -
      VAIRIN*HAIRIN)/LA(I+1)
IF (TFLAG.EQ.2) THEN
   T(I+1) = TBOT
   GOTO 110
ELSE
   CONTINUE
ENDIF
   CALL TLIQ(xa(i+1),HLIQ(I+1),T(I+1))
110 CONTINUE
125 FORMAT (1X,I3,F10.5,F9.5,2X,F6.2,F8.1,F8.1)
PRINT 125, I, YA(I), XA(I+1), T(I), VA(I), LA(I+1)
IF (XA(I+1).LT.XT.AND.KFLAG.EQ.0) THEN
   PLATES = I - 1 + (XA(I)-XT)/(XA(I)-XA(I+1))
   TTOP = T(I) + (T(I+1)-T(I))*(XA(I)-XT)/(XA(I)-
      XA(I+1))
   KFLAG = 1
   GOTO 130
ELSE
   CONTINUE
ENDIF
130 IF((XA(I)-XA(I+1).LT.0.0001) GOTO 140
   IF ((XA(I+1)-XEND).GT.FINCON) THEN
      I = I + 1
      GOTO 100
ELSE
   CONTINUE
ENDIF
140 CONTINUE
PRINT
150 FORMAT (1X,'NUMBER OF THEORETICAL
   PLATES =',F7.3)
PRINT 150, PLATES
160 FORMAT (IX,'INLET LIQUID TEMPERATURE
   =',F7.3)
PRINT 160, TTOP
170 END
C
   subroutine equila (x,tsoln,y)
   real xwat1(13),xwat2(11),slope(11),yint(13),bs(11),
      cs(11), ds(11),
   * by(13),cy(13),dy(13)
   real x,w,tdew,tdewk,tsoln,pt,psat,m,b
   integer n, j
   character flag*4
c
c  this data adapted from kohl and reisenfeld, figure11.11,
   pg. 595
c
   data xwat1/0.0025,0.0042,0.0083,0.0164,0.05,0.0776,
      0.10,0.2049,
   * 0.3049,0.4808,0.6757,0.7813,0.8929/
   data yint/-107.8,-105.3,-95.4,-88.2,-69.0,-61.6,-
      56.0,-43.0,-34.3
   * ,-24.5,-14.2,-9.0,-3.6/
   data xwat2/0.0025,0.0042,0.0083,0.0164,0.0402,
      0.02049,0.3049,
   * 0.4808,0.6757,0.7813,0.8929/
   data slope/0.4962,0.5107,0.5143,0.5393,0.5654,
      0.7414,0.825,
   * 0.9091,0.955,0.9677,0.9882/
c
   pt=101235.
   if (flag.eq.'done') goto 2
   n = 13
   call spline (n, xwat1, yint, by, cy, dy)
   j = 11
   call spline (j, xwat2, slope, bs, cs, ds)
   flag = 'done'
c  all temp in deg F
   2m = seval (j, x, xwat2, slope, bs, cs, ds)
   b = seval (n, x, xwat1, yint, by, cy, dy)
   tdew = tsoln*m + b
   tdewk - (tdew - 32.)*5./9. + 273.15
```

```
c  Maclaine-cross 1974 correlation for sat'n pressure of
     water vapor
c  all pressures in Pa
   if (tdewk .lt. 273.15) then
      psat = exp(28.87 - 6133.8/tdewk)
   else
      psat = exp(23.282-3780.82/tdewk-225805./
         tdewk**2)
   endif
c absolute humidity level w (mol H20/mol dry air)
      w = 0.622*psat/(pt-psat)*28.97/18.02
      y = w/(1. + w)
c 10 format (f5.3,1x,f5.1,1x,f8.1,1x,f6.3,1x,f7.3,1x,
      f6.1,1x,f6.1,
c  * 1x,f7.1,1x,f7.5,1x,f5.3)
c  write (6,10) x,tsoln, pt,m,b,tdew,tdewk,psat,w,y
   return
   end
C
   subroutine tliq (x,h,t)
   real a,c,d,htsln,htsnmet,h,hmet,x,tk,t,aa,bb,cc
c  A,B,C are coefficients for specific heat variation of
      water and TEG
c  resulting units are J/kmol/K
      data a/7.59e4/,c/1.538e5/,d/587./,htsln/1549.7/,ref/
         273.15/
   hmet=h*1055/.454
   htsnmet=htsln*1055/.454
c  aa,bb,cc are all coefficients in quadratic formula
      aa=(1.0-x)*d/2.0
      bb=x*a + (1.0-x)*c
      cc=-(x*a*ref + (1.0-x)*c*ref + (1.0-x)*d/
         2.0*ref**2 + hmet
   * + x*htsnmet)
c  units of TK are Kelvin
   tk=(-bb+sqrt(bb**2-4.*aa*cc))/2./aa
c  units of T are deg F
   t=(tk-273.15)*9./5.+32.0
c  10 format
(f10.1,1x,f10.1,1x,f8.1,1x,f10.1,1x,f13.1,1x,f6.1,1x,f6.1)
c  write (6,10) hmet,htsnmet,aa,bb,cc,tk,t
    return
   end
C
   SUBROUTINE MIXENTH (y,T,hmix)
c  Y is vapor mole fraction of water in air, T is mixture
      temperature
c  in degrees F; HAIR, HTVAPN, HH2OVAP, and
      HMIX all in BTU/lbmole.
c  Assumption regarding temperature of mixture is
      implemented from the
c  main program by passing the desired temperature to
      this subroutine.
      REAL y,T,kel,hair,htvapn,hh2ovap,hmix,
         a,b,c,d,e,f,g,h,i
      KEL =(T-32.)*5./9. + 273.15
      DATA A/1.04195/,B/-2.63541E-4/,C/4.84486E=7/
      HAIR = (1.-Y)*(A*(KEL-273.15) + B/2.*
         (KEL**2-273.15**2)
      * +C/3.*(KEL**3-273.15**3))*12.4667
      DATA D/2652.15/,E/.616305/,F/-4.4788E-3/
      HTVAPN = (A + B*KEL + C*KEL**2)*7.7546
      DATA G/5.31409/,H/-7.20017E-3/,I/1.14153E-5/
      HH2OVAP = Y*(G*KEL-273.15) + H/2.*
         (KEL**2-273.15**2)
      *  + I*(KEL**3-273.15**3))*7.7546 +Y*HTVAPN
      HMIX = HAIR + HH2OVAP
      return
      end
C
   SUBROUTINE SPLINE (N, X, Y, BY, CY, DY)
   INTERGER N,NM1,IB,I
   REAL X(N),Y(N),BY(N),CY(N),DY(N)
   REAL TY
   NM1=N-1
   IF (N.LT.2) RETURN
   IF (N.LT.3) GOTO 50
   DY(1) = X(2)-X(1)
   CY(2) = (Y(2)-Y(1)/DY(1)
   DO 10 I=2, NM1
      DY(I) = X(I+1)-X(I)
      BY(I) = 2.*(DY(I-1)+DY(I))
      CY(I+1) = (Y(I+1)-Y(I))/DY(I)
      CY(I) = CY(I+1)-CY(I)
   10 CONTINUE
      BY(1) = -DY(1)
      BY(N) = -DY(N-1)
      CY(1) = 0.
      CY(N) = 0.
      IF (N.EQ.3) GOTO 15
      CY(1) = CY(3)/(X(4)-X(2)) - CY(2)/(X(3)-X(1))
      CY(N) = CY(N-1)/(X(N)-X(N-2))-CY(N-2)/(X(N-
         1)-X(N-3))
      CY(1) = CY(1)*DY(1)**2/(X(4)-X(1))
      CY(N) = -CY(N)*DY(N-1)**2/(X(N)-X(N-3))
   15 DO 20 I=2,N
      TY =DY(I-1)/BY(I-1)
      BY(I) = BY(I)-TY*DY(I-1)
      CY(I) = CY(I)-TY*CY(I-1)
   20  CONTINUE
      CY(N) = CY(N)/BY(N)
      DO 30 IB=1,NM1
         I = N-IB
         CY(I) = (CY(I)-DY(I)*CY(I+1)/BY(I)
   30 CONTINUE
      BY(N) = Y(N)-Y(NM1))/DY(NM1) +
         DY(NM1)*(CY(NM1)+2.*CY(N))
      DO 40 I = 1,NM1
```

```
      BY(I) = (Y(I+1)-Y(I))/DY(I) -
         DY(I)*(CY(I+1)+2.*CY(I))
      DY(I) = (CY(I+1)-CY(I))/DY(I)
      CY(I) = 3.*CY(I)
   40 CONTINUE
      CY(N) = 3.*CY(N)
      DY(N) = DY(N-1)
      RETURN
   50 BY(1) = (Y(2)-Y(1))/(X(2)-X(1))
      CY(1) = 0.
      DY(1) = 0.
      BY(2) = BY(1)
      CY(2) = 0.
      DY(2) = 0.
      RETURN
      END
```

```
      REAL FUNCTION SEVAL (N,U,X,Y,B,C,D)
      INTERGER N
      REAL U, X(N), Y(N), B(N), C(N), D(N)
      INTERGER I, J, K
      REAL DX
      DATA I/1/
      IF (I.GE.N) I = 1
      IF (U.LT.X(I)) GOTO 10
      IF (U.LE.X(I+1) GOTO 30
   10 I = 1
      J = N+1
   20 K = (I+J)/2
      IF (U.LT.X(K)) J = K
      IF (U.GE.X(K)) I = K
      IF (J.GT.I+1) GOTO 20
   30 DX = U-X(I)
      SEVAL = Y(I)+DX*(B(I)+DX*(C(I)+DX*D(I)))
      RETURN
      END
```